Bayesian Estimation and Sensitivity Analysis for Radiative Transfer Models

Marian Farah[1], Athanasios Kottas[1], and Robin Morris[2,1], Roberto Furfaro[3], Barry Ganapol[3]

[1]Applied Math and Statistics, UC Santa Cruz, [2]USRA, [3]University of Arizona

Abstract

A Radiative Transfer Model (RTM) simulates the interaction of light with a medium. We are interested in RTMs that model light reflected from a vegetated region. We study the Leaf Canopy Model (LCM) RTM, which was designed to explore the feasibility of observing leaf chemistry remotely. The inputs to the LCM are leaf chemistry variables (chlorophyll, water, lignin, cellulose) and canopy structural parameters (leaf area index (LAI), leaf angle distribution (LAD), soil reflectance, sun angle), and the output is the upwelling radiation at the top of the canopy. In this work, we address the following question: which of the inputs to the RTM has the greatest impact on the computed observation? To answer this question, we employ a Bayesian Gaussian Process approximation to the LCM output using Markov Chain Monte Carlo (MCMC) simulation. Then, we analyze the "main effects" of the inputs to the LCM in terms of the sensitivity of the LCM's output to each of the inputs. We apply this method to 7 inputs and output obtained at 667 nm and 1640 nm wavelengths, which are associated with MODIS (a key instrument aboard the Terra and Aqua satellites) spectral bands that are sensitive to vegetation.

Introduction

- The LCM was developed in order to capture the essential biophysical processes associated with the interaction between light and vegetation by combining two different radiative transfer algorithms.
- LEAFMOD simulates the radiative regime inside the single leaf, and CANMOD combines the information coming from LEAFMOD with canopy structural parameters to compute the radiative regime within and at the top of the canopy.

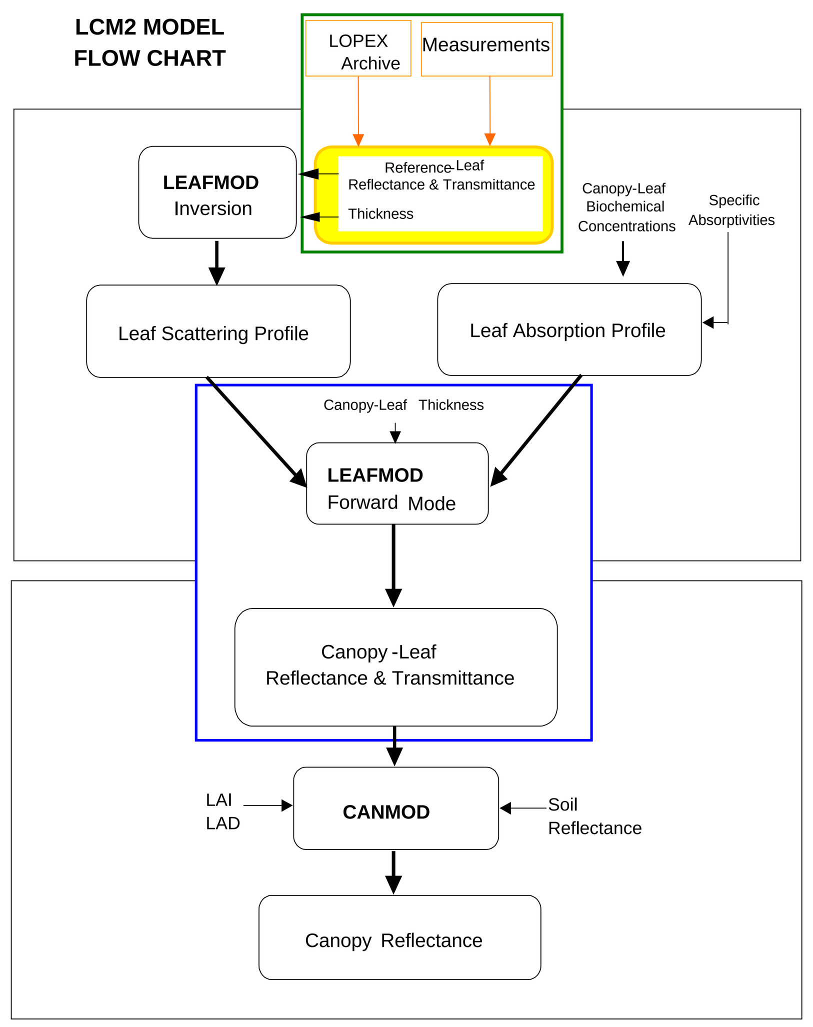

Figure 1: Flow chart demonstrating the operations of the coupled algorithm of the LCM

- The LAD variable is set to planophile (leaves mostly horizontal), and the sun angle is set to zenith.
- **Input variables**: Chlorophyll, water, thickness, lignin, protein, LAI, and soil reflectance.
- **Output**: $y = f(\boldsymbol{v})$ is hemispherical reflectance, which is the LCM output to the inputs listed above and denoted by $\boldsymbol{v} = (v_1, v_2, \ldots, v_7)$.

Global Sensitivity Analysis

- Output function Decomposition:

$$y = f(\boldsymbol{v}) = E(y) + \sum_{i=1}^{7} z_i(v_i) + \sum_{i<j} z_{i,j}(v_i, v_j) + \cdots + z_{1,2,\ldots,7}(v_1, v_2, \ldots, v_7) \quad (1)$$

- The global mean is given by $E(y) = \int_{\boldsymbol{v}} f(\boldsymbol{v})\, dH(\boldsymbol{v})$, where $H(\boldsymbol{v})$ is the distribution of the inputs. Based on related literature, we use independent uniforms over the ranges of the inputs.
- The main effects are given by $z_i(v_i) = E(y|v_i) - E(y) = \int_{\boldsymbol{v}_{-i}} f(\boldsymbol{v})\, dH(\boldsymbol{v}_{-i}|v_i) - E(y)$, where $\boldsymbol{v}_{-i}$ denotes all the elements of $\boldsymbol{v}$ except v_i.
- The later terms of the decomposition are the interactions, which give the combined influence of two or more inputs taken together.
- Computing the main effects requires the evaluation of multidimensional integrals over the input space of the model, and evaluating RTMs can be computationally expensive.
- We use a Gaussian Process (GP) approximation to the RTM output, a technique known in statistical literature as ***emulation***. This approximation allows for evaluating the main effects analytically.

Bayesian Model for the Gaussian Process

- A GP is a stochastic process that generates a collection of random variables, any finite number of which have a multivariate normal distribution.
- Given the input $\boldsymbol{v} = (v_1, v_2, \ldots, v_7)$, a GP, $f(\boldsymbol{v})$, is fully specified by its mean function, $\mu(\boldsymbol{v})$, and covariance function, $C(\boldsymbol{v}, \boldsymbol{v}') = \tau^2 R(|\boldsymbol{v} - \boldsymbol{v}'|)$, which is taken to be isotropic with constant variance τ^2 and a correlation function, $R(|\boldsymbol{v} - \boldsymbol{v}'|)$.
- Consider the exponential correlation function:

$$R(|\boldsymbol{v} - \boldsymbol{v}'|) = \exp\left\{ -\sum_{j=1}^{7} \phi_j |v_j - v_j'| \right\}, \text{ where } \phi_j > 0. \quad (2)$$

- Assume the data, $D = \{y_i, \boldsymbol{x_i} = (x_{i1}, x_{i2}, \ldots, x_{i7}) : i = 1, 2, 3, \ldots, n\}$, are a sample from a GP (i.e. we are approximating the function $y = f(\boldsymbol{v})$ by a GP).
- We place priors on the parameters of the GP, μ, τ^2, and ϕ_j, for $j = \{1, 2, \ldots, 7\}$, as follows.

$$\mu \sim N(a_\mu, b_\mu) \qquad \tau^2 \sim \text{Inv.Gamma}(a_\tau, b_\tau) \qquad \phi_j \sim \text{Unif}\left(0, b_{\phi_j}\right) \quad (3)$$

- Using MCMC simulation, we obtain samples of $P(\boldsymbol{\theta}, \mu, \tau^2, \boldsymbol{\phi}|D)$, which is the joint posterior distribution of μ, τ^2, $\boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_7)$, and $\boldsymbol{\theta} = (f(\boldsymbol{x}_1), f(\boldsymbol{x}_2), \ldots, f(\boldsymbol{x}_n))$.
- Calculating the main effects requires computing $E^*\{E(y|v_i)|D\}$ and $E^*\{E(y)|D\}$, where $E^*\{\cdot|D\}$ indicates the expectations with respect to the GP posterior predictive distributions.

$$E^*\{E(y)|D\} = \int \left(\mu + T^T R^{-1}(\boldsymbol{\theta} - \mu \mathbf{1}_n)\right) dP\left(\boldsymbol{\theta}, \mu, \tau^2, \boldsymbol{\phi}|D\right). \quad (4)$$

And for each value u_j of the j–th input, we have:

$$E^*\{E(y|u_i)|D\} = \int \left(\mu + T_j^T(u_j) R^{-1}(\boldsymbol{\theta} - \mu \mathbf{1}_n)\right) dP\left(\boldsymbol{\theta}, \mu, \tau^2, \boldsymbol{\phi}|D\right), \quad (5)$$

where T and $T_j(u_j)$ are $n \times 1$ vectors that are functions of the input space and of $\boldsymbol{\phi}$, and R is the observed correlation matrix.

Some Results

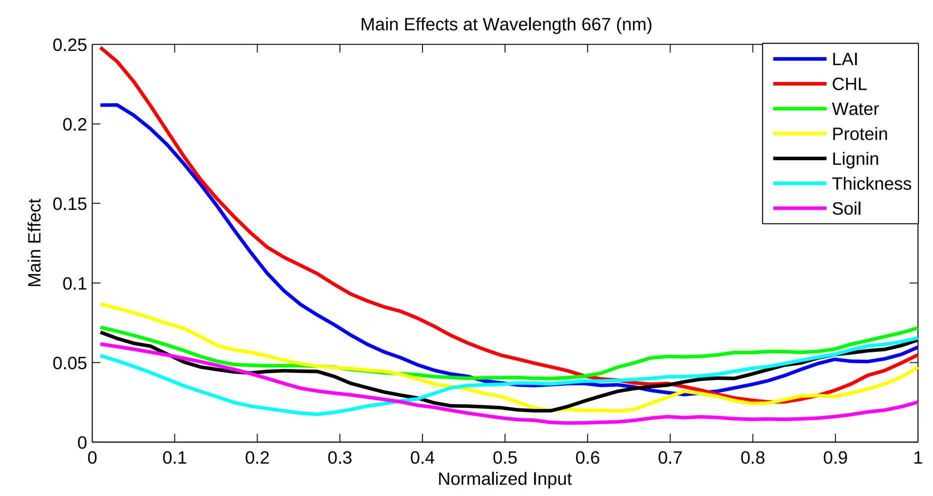

Figure 2: The main effects for the LCM at wavelength 667 (nm).

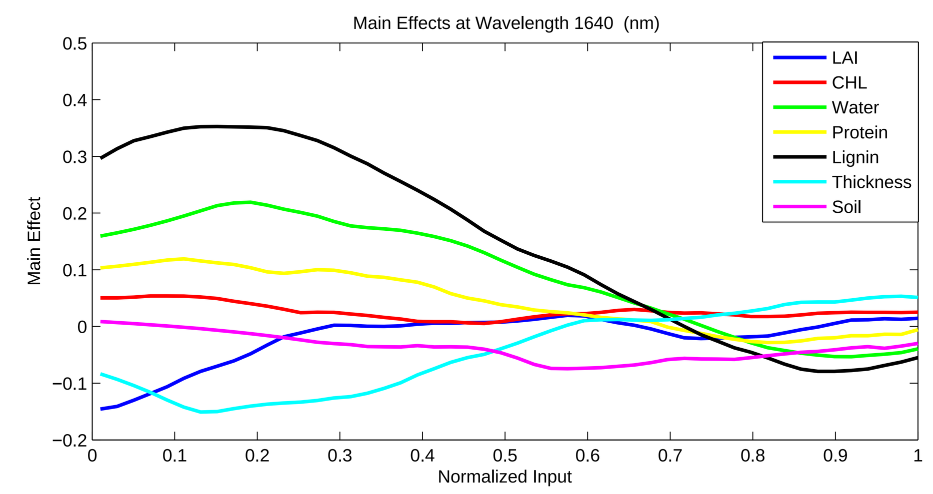

Figure 3: The main effects for the LCM at wavelength 1640 (nm).

- The slope of each main effect gives information as to whether the output is an increasing or decreasing function of that input.
- For example, at wavelength 667, the LCM is most sensitive to LAI and chlorophyll, which have nonlinear effects, and an increase in LAI or chlorophyll produces a decrease in reflectance.

Discussion and Future Work

- We have implemented a Bayesian approach, via MCMC methods for the GP emulator, to obtain point estimates for all the main effects associated with the 7 inputs. To quantify the uncertainty introduced by the GP approximation of the LCM, we will obtain $Var^*\{E(y|v_i)|D\}$.
- Using a fully Bayesian approach, we will obtain distributions (rather than point estimates) of the main effects associated with the 7 inputs at 8 MODIS bands as well as "sensitivity indices", which give a measure of how much of the variance of the output is due to each input.
- We will also develop a hierarchical Bayesian model accounting for all 4 LAD classifications using a hierarchical GP formulation for the corresponding output functions $f_j(\boldsymbol{v})$, for $j = 1, 2, 3, 4$.

Acknowledgements:

This work was supported by the NASA AISR program through grant number NNX07AV69G.